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Eu(3+)

20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

Previously reported spectra of the pentaphosphates of Nd^{3+} and Eu^{3+} are analyzed by diagonalizing a parametrized $C_s(C_{1h})$ Hamiltonian in free-ion bases involving the five and seven lowest J-multiplets, respectively, of each ion. By reassigning symmetries to the reported Eu levels according to predictions from scaled crystal field parameters, B_{km}, that fit 28 Nd^{3+} levels to

next page

B sub km

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/cm Eu(3+)

cont 7.61 cm^{-1}, a fit of 10.43 cm^{-1} to 46 Eu^{3+} levels is obtained. Predicted B_{km} and energy levels for all the lanthanide pentaphosphates are then obtained.

B sub km

CONTENTS

TABLES

TABLES (Cont'd)

1. INTRODUCTION

Interest in new materials that have potentially good laser properties has recently been focused on the rare-earth pentaphosphates.[1] The apparent lack of quenching between the active ions in these materials, as evidenced by the sharp lines observed even when there is 100-percent doping as in NdP_5O_{14}, leads to the obvious expectation of producing smaller laser crystals with these materials.

In this work, previously reported spectra of the pentaphosphates of Nd and Eu were analyzed by diagonalizing a parametrized $C_s(C_{1h})$ Hamiltonian in free-ion bases involving the five and seven lowest J-multiplets, respectively, of each ion. By reassigning symmetries to the reported[2] Eu levels according to predictions from scaled crystal field parameters, B_{km}, that fit 28 Nd levels[3] to 7.61 cm^{-1}, a fit of 10.43 cm^{-1} to 46 levels of Eu was obtained. Predicted B_{km} and energy levels for all the lanthanide pentaphosphates also were obtained.

2. CALCULATIONS

The point group symmetry at the rare-earth ion site[4,5] is C_1 which gives rise to the crystal field Hamiltonian

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[1] *H. G. Danielmeyer and H. P. Weber, IEEE J. Quantum Electron., QE-8 (1972), 805.*

[2] *C. Brecher, J. Chem. Phys., 61 (1974), 2297.*

[3] *M. Blatte, H. G. Danielmeyer, and R. Ulrich, Appl. Phys., 1 (1973), 275.*

[4] *H. Y-P Hong, Acta Crystallogr., B30 (1974), 468.*

[5] *K.-R. Albrand, R. Attig, J. Fenner, J. P. Jeser, and D. Mootz, Mater. Res. Bull., 9 (1974), 129.*

$$H_x = \Sigma B_{km} C_{km} \, , \; k = 2, 4, 6 \, , \tag{1}$$

where $|m| \le k$ and B_{km} for $m \neq 0$ may be complex. This Hamiltonian represents the lowest possible symmetry in the electrostatic potential at the rare-earth site, and it contains 26 independent B_{km}, counting real and imaginary parts of the B_{km}. In order to obtain a manageable representation for the crystal field that may be extended to predict spectra of all the lanthanide pentaphosphates, we assume the B_{km} with $m = \pm$ odd integer to be negligible (subject to justification at a later date). The resulting Hamiltonian given by equation (1) with the added restriction

$$m = 0, \pm 2, \ldots, \pm k \tag{2}$$

results in 14 independent parameters and has the appearance of $C_s (C_{1h})$ symmetry.

This Hamiltonian was diagonalized in free-ion bases by using the lowest five and seven J-multiplets, respectively, of Nd and Eu, and the B_{km} and multiplet centroids were varied to fit reported spectra for NdP_5O_{14}[3] and EuP_5O_{14}.[2] To begin the analysis, the B_{km} of Brecher[2] were converted from the form[6] $A_k^m \langle r^k \rangle$ to the B_{km} of equation (1). These B_{km}, given in table I, line 1, were then used to calculate theoretical energy levels for the ^7F term of Eu. Crystal quantum numbers $\mu = 0, 1$ were assigned to experimental energy levels according to which theoretical level each approximated. By maintaining these assignments, the B_{km} and

[2] *C. Brecher, J. Chem. Phys., 61 (1974), 2297.*

[3] *M. Blatte, H. G. Danielmeyer, and R. Ulrich, Appl. Phys., 1 (1973), 275.*

[6] *A. J. Kassman, J. Chem. Phys., 53 (1970), 4118.*

centroids were varied to give a best fit of 14.6 cm^{-1} for 49 levels with the B_{km} of table I, line 2. These B_{km} were then scaled according to the ratios[7]

$$B_{km}(Nd)/B_{km}(Eu) = 1.024,\ 1.194,\ 1.271;\ k = 2, 4, 6\ , \tag{3}$$

and used as starting parameters to fit the 28 levels of the ^4I term and $^4F_{3/2}$ multiplet of Nd. A fit of 7.6 cm^{-1} was obtained with the B_{km} of table I, line 4.

Since the final B_{km} for Nd differed significantly from the initial set, they were then scaled back to Eu to determine if new crystal quantum number assignments to the Eu levels would result in a better fit. By maintaining the new assignments, a second set of B_{km} given in table I, line 3, was obtained that gave a fit of 13.2 cm^{-1}, better than the 14.6 cm^{-1} resulting from Brecher's assignments, but not as good a fit as the Nd spectrum. Three experimental levels at 1928, 4952, and 4993 cm^{-1} differed by more than 30 cm^{-1} from theoretical values in the best-fit calculation for Eu. If they are ignored, the 13.2-cm^{-1} fit for 49 levels is reduced to a 10.4-cm^{-1} fit without any further refitting of the B_{km} to the remaining 46 levels.

Comparing the final parameters for Eu in table I, line 3, with those of Nd in line 4, it is not clear what the best way is of extending the results to all the lanthanides. There is some consistency between the parameters, however, if one compares the rotational invariants $B_{oo}(k, N)$ for each ion where we define[8]

$$B_{oo}(k, N) = \left[\Sigma_m |B_{km}(N)|^2\right]^{1/2}\ , \tag{4}$$

[7]*N. Karayianis, D. E. Wortman, and C. A. Morrison, Crystal Field Parameters for Triply Ionized Lanthanides in Yttrium Orthoaluminate, Solid State Communications* 18 *(1976), 1299.*

[8]*N. Karayianis, C. A. Morrison, and D. E. Wortman, J. Chem. Phys.,* 64 *(1976), 3890.*

TABLE I. CRYSTAL FIELD PARAMETERS, B_{km}, IN CM^{-1} FOR NdP_5O_{14} and EuP_5O_{14}

Ion	B_{20}	B_{22}	B_{40}	B_{42}		B_{44}		B_{60}	B_{62}		B_{64}		B_{66}		Multiplets (No.)	Levels (No.)	Experimental levels (No.)	Energy rms deviation (cm^{-1})
				Real	Imaginary	Real	Imaginary		Real	Imaginary	Real	Imaginary	Real	Imaginary				
Eu[a]	-508	167	648	146	0	-847	0	195	74	0	75	0	-401	0	7	49	49	18.94
Eu[b]	-453	270	720	114	100	-799	49	245	97	-41	-22	-257	-424	-16	7	49	49	14.56
Eu[c]	-586	213	-83	751	80	111	-184	132	-118	388	81	-68	-457	-3	7	40	49 46	13.18 10.43
Nd[d]	-785	16	-219	-661	149	-621	52	291	-242	-275	249	-391	18	-176	5	28	28	7.61

[a] *Brecher's parameters with J-mixing included and centroids adjusted for best rms fit (C. Brecher, J. Chem. Phys.,* 61 *(1974), 2297).*
[b] *Best* B_{km} *fitting levels with crystal quantum number assignments from calculation of line 1.*
[c] *Best* B_{km} *fitting levels with crystal quantum number assignments starting with* B_{km} *scaled from line 4.*
[d] *Best* B_{km} *starting with* B_{km} *scaled from line 2.*

and N represents the configuration f^N of the particular lanthanide. Table II gives the quantities $B_{oo}(k, 3)$ and $B_{oo}(k, 6)$ calculated for Nd and Eu, respectively, by using their final B_{km} values from table I. These quantities tend toward lower values as N gets larger. To derive B_{km} for all the lanthanides, we defined[8] average constants η_{km} independent of N by

$$\eta_{km} = \frac{1}{2}\left[\frac{|B_{km}(Nd)|}{B_{oo}(k, 3)} + \frac{|B_{km}(Eu)|}{B_{oo}(k, 6)}\right], \tag{5}$$

chose expressions for the $B_{oo}(k, N)$ and phases $\phi_{km}(N)$ linear in N* to fit the values in tables II and I, respectively, and calculated B_{km} for all the lanthanides by

$$B_{km}(N) = \eta_{km}\, B_{oo}(k, N)\, \exp\left[i\phi_{km}(N)\right] . \tag{6}$$

The parameters given by equation (6) were reported elsewhere.[8] A simpler method was used here, however, to obtain the B_{km} for the lanthanides. This method consists of deriving a set of B_{km} such that

$$B_{km}(N) = B_{km}(x) + \rho_k(N)/\rho_k(x) \tag{7}$$

for x = Nd and then for x = Eu; the ρ_k are from table II by Karayianis et al.[7] The resulting B_{km} were then averaged, and these parameters are given in table III.

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*N is the number of equivalent 4f electrons specifying the electronic configuration for that ion. N = 2 for Pr, 3 for Nd, etc.

[7]N. Karayianis, D. E. Wortman, and C. A. Morrison, *Crystal Field Parameters for Triply Ionized Lanthanides in Yttrium Orthoaluminate*, Solid State Communications 18 (1976), 1299.

[8]N. Karayianis, C. A. Morrison, and D. E. Wortman, J. Chem. Phys., 64 (1976), 3890.

TABLE II. ROTATIONAL INVARIANTS $B_{00}(k, N) = (\Sigma_m |B_{km}(N)|^2)^{1/2}$ FOR NdP_5O_{14} AND EuP_5O_{14}

	Nd	Eu
k	$B_{00}(k,3)^a$	$B_{00}(k,6)^b$
2	785	659
4	1320	1114
6	920	887

[a] Calculated from table I, line 4.
[b] Calculated from table I, line 3.

Energy levels calculated by using the B_{km} of tables I and III for the lowest-lying six to eight multiplets of the lanthanide pentaphosphates are given in tables IV to XVI.

In order to make intensity calculations, some estimates of the odd-fold (odd-k) crystal field components (A_{km}) are necessary. These can be obtained by appropriate lattice sums.[9] In this work, we have performed the lattice sums for NdP_5O_{14} using the x-ray data of Hong[4] for oxygen charges $q_0 = -1$ and -2; the results are given in table XVII. The one fold field, A_{1m}, is not expected to be accurate because of its slow convergence. By appropriate rotations of the coordinate system chosen for the calculation of the A_{km} of table XVII, different sets of A_{km} can be generated. Since the A_{km} are linear functions of q_0, a value of q_0 can be chosen by using the relation $B_{km} = \rho_k A_{km}$ and the ρ_k (reported in table II by Karayianis[7]) to obtain a best fit of calculated B_{km} to phenomenological B_{km}.

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[4] H. Y-P Hong, *Acta Crystallogr.*, B30 (1974), 468.

[7] N. Karayianis, D. E. Wortman, and C. A. Morrison, *Crystal Field Parameters for Triply Ionized Lanthanides in Yttrium Orthoaluminate*, Solid State Communications 18(1976), 1299.

[9] N. Karayianis and C. A. Morrison, *Rare Earth Ion-Host Lattice Interactions 1. Point Charge Lattice Sum in Scheelites*, Harry Diamond Laboratories TR-1648 (October 1973).

TABLE III. ESTIMATED CRYSTAL FIELD PARAMETERS, B_{km}, IN CM^{-1} FOR LnP_5O_{14} (SPACE GROUP $P2_{1/c}$) WHERE Ln IS ONE OF THE LANTHANIDES

Ion	B_{20}	B_{22}	B_{40}	B_{42}		B_{44}		B_{60}	B_{62}		B_{64}		B_{66}		rms cm^{-1}	Table No.
				Real	Imaginary	Real	Imaginary		Real	Imaginary	Real	Imaginary	Real	Imaginary		
Pr	-780	158	-164	-621	-536	-152	-474	240	-338	205	156	-312	210	-301	-	IV
Nd	-755	153	-159	-773	174	-479	40	235	-256	-290	183	-288	36	-357	9.739[a]	VI
Pm	-729	148	-153	-307	698	-66	459	230	236	-295	208	-261	-139	-322	-	VII
Sm	-703	142	-147	364	636	415	160	224	324	176	228	-232	-272	-209	-	VIII
Eu	-675	137	-140	696	82	238	-353	218	-114	341	245	-202	-330	-49	[b]	X
Gd	-646	131	-134	457	-487	-277	-296	213	-346	-52	258	-171	-304	115	-	XI
Tb	-616	125	-127	-114	-623	-332	193	207	-9	-340	267	-139	-204	242	-	XII
Dy[c]	-584	118	-119	-535	-262	107	346	201	324	-66	271	-107	-59	301	-	XIII
Ho[c]	-551	112	-111	-494	257	337	-25	194	118	297	272	-76	92	283	-	XIV
Er[c]	-515	104	-103	-81	508	47	-308	188	-263	162	269	-45	211	195	-	XV
Tm[c]	-477	97	-94	328	334	-264	-105	181	-198	-222	263	-16	269	65	-	XVI

[a] *Fit to data of C. Brecher, J. Chem. Phys., 61 (1974), 2297.*
[b] *Fit to data of table I, lines 1 and 2.*
[c] *These lanthanides have not been grown in the $P2_{1/c}$ space group structure.*

TABLE IV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR PrP_5O_{14}

```
PR IN PRP5014.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.   9/24/75.
INIT.  BKM AND CENTROIDS.   0 = -0.000
   -779.700 = B20      158.100 = B22     -164.300 = B40     -620.700 = B42     -536.400 = B42
    240.100 = B60     -337.700 = B62      205.400 = B62      155.700 = B64     -312.400 = B64
3H 4          251.0
3H 5         2354.0     -151.600 = B44     -474.500 = B44
3H 6         4527.0      210.500 = B66     -300.700 = B66
3F 2         5101.0
3F 3         6478.0
3F 4         6950.0
1G 4         9923.0
1D 2        16802.0
```

FREE ION		PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	3H 4	99.6	2	-65.1	0.0
2	3H 4	99.3	0	-14.6	0.0
3	3H 4	99.5	0	70.4	0.0
4	3H 4	99.4	2	203.3	0.0
5	3H 4	99.5	2	243.6	0.0
6	3H 4	99.5	0	305.3	0.0
7	3H 4	99.6	2	333.9	0.0
8	3H 4	99.2	0	489.7	0.0
9	3H 4	99.5	0	523.4	0.0
10	3H 5	99.1	2	2077.1	0.0
11	3H 5	99.0	0	2085.7	0.0
12	3H 5	98.7	0	2183.9	0.0
13	3H 5	98.9	2	2238.3	0.0
14	3H 5	99.1	2	2295.7	0.0
15	3H 5	99.0	0	2387.1	0.0
16	3H 5	99.2	2	2397.7	0.0
17	3H 5	98.7	0	2407.4	0.0
18	3H 5	99.2	0	2440.9	0.0
19	3H 5	98.8	2	2598.7	0.0
20	3H 5	99.4	2	2617.1	0.0
21	3H 6	98.7	2	4177.9	0.0
22	3H 6	98.9	0	4178.3	0.0
23	3H 6	97.7	0	4310.5	0.0
24	3H 6	98.4	2	4351.9	0.0
25	3H 6	98.7	2	4416.8	0.0
26	3H 6	98.4	0	4484.4	0.0
27	3H 6	98.2	0	4515.7	0.0
28	3H 6	97.1	2	4590.2	0.0
29	3H 6	98.1	0	4617.2	0.0
30	3H 6	98.5	2	4631.3	0.0
31	3H 6	97.6	2	4667.8	0.0
32	3H 6	92.2	0	4812.9	0.0
33	3H 6	95.8	0	4829.7	0.0
34	3F 2	94.5	0	5060.7	0.0
35	3F 2	97.1	0	5070.0	0.0
36	3F 2	96.7	2	5146.3	0.0
37	3F 2	97.2	2	5172.2	0.0
38	3F 2	92.9	0	5220.3	0.0
39	3F 3	96.1	2	6402.9	0.0
40	3F 3	98.3	2	6445.1	0.0
41	3F 3	96.0	0	6474.1	0.0
42	3F 3	97.6	2	6512.6	0.0
43	3F 3	96.1	0	6514.0	0.0
44	3F 3	98.9	2	6555.9	0.0
45	3F 3	94.8	0	6570.0	0.0
46	3F 4	97.3	0	6819.3	0.0
47	3F 4	95.1	0	6866.8	0.0
48	3F 4	94.9	2	6896.4	0.0

TABLE IV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR PrP_5O_{14} (Cont'd)

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
49 3F 4	99.2	2	6929.0	0.0
50 3F 4	99.3	2	7002.0	0.0
51 3F 4	96.7	0	7029.3	0.0
52 3F 4	98.7	0	7043.4	0.0
53 3F 4	98.4	2	7072.7	0.0
54 3F 4	98.0	0	7091.4	0.0
55 1G 4	99.5	0	9647.3	0.0
56 1G 4	99.8	2	9787.5	0.0
57 1G 4	99.9	0	9790.4	0.0
58 1G 4	99.9	2	9863.4	0.0
59 1G 4	99.9	2	9950.7	0.0
60 1G 4	99.9	0	9965.6	0.0
61 1G 4	99.9	0	10080.2	0.0
62 1G 4	99.8	2	10129.5	0.0
63 1G 4	99.7	0	10157.1	0.0
64 1D 2	100.0	0	16523.0	0.0
65 1D 2	99.9	2	16742.3	0.0
66 1D 2	100.0	0	16748.9	0.0
67 1D 2	99.9	0	16961.4	0.0
68 1D 2	100.0	2	17069.0	0.0

TABLE V. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS, B_{km}, for Nd^{3+} in NdP_5O_{14}[a]

```
ND IN ULTRA PHOS BLATTE ET AL DATA.  HOME OVER NITE OF SEPT. 18, 1975.
FINAL  BKM AND CENTROIDS.  Q =   7.609
   -785.211 = B20      16.203 = B22     -216.583 = B40     -661.206 = B42      148.620 = B42
    290.619 = B60    -242.267 = B62     -274.634 = B62      248.941 = B64     -391.441 = B64
4I 9/2        182.7
4I11/2       2055.4   -620.883 = B44       51.669 = B44
4I13/2       4036.3     18.127 = B66     -175.697 = B66
4I15/2       6083.5
4F 3/2      11523.6
FREE ION   PCT PURE  2MU  THEO.ENERGY  EXP.ENERGY
 1 4I 9/2       99.6    1        -8.4        0.0*
 2 4I 9/2       99.4    1        86.3       82.0
 3 4I 9/2       99.4    1       195.4      207.0*
 4 4I 9/2       99.6    1       258.3      256.0
 5 4I 9/2       99.7    1       329.3      317.0*

 6 4I11/2       99.4    1      1956.6     1958.0
 7 4I11/2       99.1    1      1981.3     1982.0
 8 4I11/2       99.1    1      2035.1     2044.0*
 9 4I11/2       99.2    1      2075.9     2062.0*
10 4I11/2       99.3    1      2104.5     2097.0
11 4I11/2       99.4    1      2166.3     2178.0*

12 4I13/2       99.5    1      3917.6     3914.0
13 4I13/2       99.2    1      3945.2     3943.0
14 4I13/2       99.1    1      3997.8     3995.0
15 4I13/2       99.6    1      4032.5     4037.0
16 4I13/2       99.1    1      4078.0     4090.0*
17 4I13/2       99.5    1      4116.9     4106.0*
18 4I13/2       99.5    1      4166.7     4171.0

19 4I15/2       99.4    1      5871.4     5872.0
20 4I15/2       99.6    1      5910.9     5912.0
21 4I15/2       99.6    1      6019.1     6011.0*
22 4I15/2       99.8    1      6065.0     6072.0
23 4I15/2       99.6    1      6094.4     6081.0*
24 4I15/2       99.8    1      6207.1     6210.0
25 4I15/2       99.9    1      6264.0     6274.0*
26 4I15/2       99.9    1      6287.8     6283.0

27 4F 3/2      100.0    1     11468.1    11473.0
28 4F 3/2      100.0    1     11587.4    11583.0


CENTROIDS, CRYSTAL =     4043.2     FREE ION =      4043.4
```

[a]*The least-rms deviation between the calculated and experimental energy levels is 7.61 cm^{-1} (M. Blatte, H. G. Danielmeyer, and R. Ulrich, Appl. Phys., 1 (1973), 275).*

TABLE VI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR NdP_5O_{14}

```
ND IN NDP5014.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.   9/24/75.
INIT.  BKM AND CENTROIDS.   Q = -0.000
   -754.900 = B20      153.000 = B22     -158.600 = B40     -772.800 = B42      174.200 = B42
    234.900 = B60     -255.500 = B62     -290.300 = B62      183.400 = B64     -288.000 = B64
4I 9/2        182.7
4I11/2       2055.4    -479.300 = B44       40.100 = B44
4I13/2       4036.3      36.500 = B66     -357.300 = B66
4I15/2       6083.5
4F 3/2      11523.6
4F 5/2      12403.0
2H 9/2 2    12670.0
4F 7/2      13476.0
4S 3/2      13583.0
4F 9/2      14760.0
```

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1 4I 9/2	99.5	1	-4.6	0.0
2 4I 9/2	99.6	1	73.8	0.0
3 4I 9/2	99.5	1	201.0	0.0
4 4I 9/2	99.4	1	256.5	0.0
5 4I 9/2	99.7	1	326.6	0.0
6 4I11/2	99.5	1	1960.3	0.0
7 4I11/2	99.2	1	1973.2	0.0
8 4I11/2	99.1	1	2031.5	0.0
9 4I11/2	99.0	1	2083.7	0.0
10 4I11/2	99.3	1	2100.7	0.0
11 4I11/2	99.5	1	2161.8	0.0
12 4I13/2	99.4	1	3920.8	0.0
13 4I13/2	99.4	1	3942.8	0.0
14 4I13/2	99.2	1	3990.3	0.0
15 4I13/2	99.3	1	4022.3	0.0
16 4I13/2	99.1	1	4086.1	0.0
17 4I13/2	99.4	1	4112.0	0.0
18 4I13/2	99.6	1	4163.5	0.0
19 4I15/2	99.4	1	5865.5	0.0
20 4I15/2	99.5	1	5921.0	0.0
21 4I15/2	99.8	1	6016.7	0.0
22 4I15/2	99.7	1	6048.4	0.0
23 4I15/2	99.5	1	6083.3	0.0
24 4I15/2	99.8	1	6212.9	0.0
25 4I15/2	99.9	1	6255.0	0.0
26 4I15/2	99.9	1	6293.3	0.0
27 4F 3/2	98.6	1	11451.7	0.0
28 4F 3/2	98.9	1	11576.6	0.0
29 4F 5/2	97.3	1	12336.0	0.0
30 4F 5/2	94.9	1	12399.8	0.0
31 4F 5/2	96.4	1	12462.0	0.0
32 2H 9/2 2	98.3	1	12577.6	0.0
33 2H 9/2 2	96.8	1	12603.0	0.0
34 2H 9/2 2	98.5	1	12678.1	0.0
35 2H 9/2 2	98.5	1	12754.5	0.0
36 2H 9/2 2	98.9	1	12755.3	0.0
37 4F 7/2	99.0	1	13370.7	0.0
38 4F 7/2	98.6	1	13475.9	0.0
39 4F 7/2	98.7	1	13493.9	0.0
40 4S 3/2	85.5	1	13579.3	0.0
41 4F 7/2	64.9	1	13589.5	0.0
42 4S 3/2	79.5	1	13593.1	0.0

TABLE VI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR NdP_5O_{14} (Cont'd)

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
43 4F 9/2	99.6	1	14655.2	0.C
44 4F 9/2	99.6	1	14711.5	0.C
45 4F 9/2	99.3	1	14793.8	0.C
46 4F 9/2	99.8	1	14837.6	0.C
47 4F 9/2	99.8	1	1485C.0	0.C

TABLE VII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR PmP_5O_{14}

```
PM IN PMP5O14.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.  9/24/75.
INIT.  BKM AND CENTROIDS.  Q = -0.000
   -729.300 = B20     147.800 = B22    -152.800 = B40    -307.400 = B42     698.300 = B42
    229.500 = B60     235.800 = B62    -295.300 = B62     207.700 = B64    -261.200 = B64
5I 4        233.0
5I 5       1731.0     -65.700 = B44     455.600 = B44
5I 6       3306.0    -138.800 = B66    -322.400 = B66
5I 7       4953.0
5I 8       6716.0
5F 1      12298.0
```

FREE ION			PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	5I	4	99.9	0	115.9	0.0
2	5I	4	99.7	2	142.6	0.0
3	5I	4	99.7	0	142.9	0.0
4	5I	4	99.4	2	153.7	0.0
5	5I	4	99.2	0	169.5	0.0
6	5I	4	98.9	2	215.2	0.0
7	5I	4	99.5	0	286.9	0.0
8	5I	4	98.5	0	355.3	0.0
9	5I	4	98.9	2	393.1	0.0
10	5I	5	99.8	2	1620.5	0.0
11	5I	5	99.6	2	1633.3	0.0
12	5I	5	98.9	0	1697.4	0.0
13	5I	5	99.3	0	1700.9	0.0
14	5I	5	99.1	2	1710.2	0.0
15	5I	5	99.3	0	1721.2	0.0
16	5I	5	98.5	2	1738.2	0.0
17	5I	5	99.0	0	1770.2	0.0
18	5I	5	98.2	2	1792.6	0.0
19	5I	5	99.6	2	1809.6	0.0
20	5I	5	98.2	0	1827.0	0.0
21	5I	6	99.7	0	3200.2	0.0
22	5I	6	99.8	0	3201.9	0.0
23	5I	6	99.4	2	3258.2	0.0
24	5I	6	99.5	2	3270.5	0.0
25	5I	6	98.9	0	3281.8	0.0
26	5I	6	99.1	2	3287.1	0.0
27	5I	6	98.7	0	3305.2	0.0
28	5I	6	98.8	2	3319.5	0.0
29	5I	6	99.1	0	3326.2	0.0
30	5I	6	99.1	0	3364.8	0.0
31	5I	6	98.6	2	3366.5	0.0
32	5I	6	99.4	0	3389.6	0.0
33	5I	6	99.4	2	3391.1	0.0
34	5I	7	99.7	2	4855.9	0.0
35	5I	7	99.8	2	4856.4	0.0
36	5I	7	99.3	0	4882.5	0.0
37	5I	7	99.8	0	4885.6	0.0
38	5I	7	99.0	2	4888.5	0.0
39	5I	7	99.2	0	4891.8	0.0
40	5I	7	99.4	2	4936.7	0.0
41	5I	7	99.4	2	4939.7	0.0
42	5I	7	98.9	0	4985.9	0.0
43	5I	7	98.9	0	4992.2	0.0
44	5I	7	99.1	2	5017.8	0.0
45	5I	7	99.0	2	5031.3	0.0
46	5I	7	99.1	0	5039.3	0.0
47	5I	7	99.1	0	5051.1	0.0
48	5I	7	99.1	2	5052.3	0.0
49	5I	8	100.0	0	6547.6	0.0
50	5I	8	100.0	2	6548.1	0.0
51	5I	8	99.9	0	6586.4	0.0
52	5I	8	99.9	2	6588.2	0.0
53	5I	8	99.8	0	6591.1	0.0
54	5I	8	99.8	2	6595.4	0.0
55	5I	8	99.8	0	6670.7	0.0
56	5I	8	99.8	0	6682.3	0.0
57	5I	8	99.7	2	6694.4	0.0
58	5I	8	99.5	2	6731.2	0.0
59	5I	8	99.5	0	6751.5	0.0
60	5I	8	99.7	2	6814.8	0.0

TABLE VII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR PmP_5O_{14}

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
61 5I 8	99.6	0	6822.5	0.0
62 5I 8	99.6	0	6891.5	0.0
63 5I 8	99.6	2	6894.5	0.0
64 5I 8	99.0	2	6944.2	0.0
65 5I 8	99.0	0	6944.8	0.0
66 5F 1	100.0	0	12241.3	0.0
67 5F 1	100.0	2	12317.9	0.0
68 5F 1	100.0	2	12346.4	0.0

TABLE VIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR SmP_5O_{14}

```
SM IN SMP5014.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.  9/24/75.
INIT.  BKM AND CENTROIDS.  0 = -0.000
   -702.700 = B20     142.400 = B22    -146.700 = B40     363.800 = B42     635.900 = B42
    224.100 = B60     323.900 = B62     176.400 = B62     228.200 = B64    -232.300 = B64
6H 5/2       134.0
6H 7/2      1183.0    415.100 = B44     160.000 = B44
6H 9/2      2398.0   -271.500 = B66    -208.900 = B66
6H11/2      3737.0
6H13/2      5098.0
6F 1/2      6355.0
6H15/2      6550.0
6F 3/2      6700.0
6F 5/2      7116.0
6F 7/2      7995.0
6F 9/2      9147.0
```

FREE ION		PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	6H 5/2	98.6	1	-52.5	0.0
2	6H 5/2	98.6	1	136.7	0.0
3	6H 5/2	98.4	1	239.4	0.0
4	6H 7/2	98.6	1	1021.4	0.0
5	6H 7/2	98.1	1	1132.7	0.0
6	6H 7/2	97.4	1	1219.0	0.0
7	6H 7/2	98.5	1	1316.3	0.0
8	6H 9/2	98.6	1	2252.6	0.0
9	6H 9/2	98.2	1	2305.3	0.0
10	6H 9/2	98.4	1	2403.2	0.0
11	6H 9/2	98.2	1	2458.7	0.0
12	6H 9/2	98.9	1	2524.6	0.0
13	6H11/2	98.9	1	3566.7	0.0
14	6H11/2	98.1	1	3634.3	0.0
15	6H11/2	98.4	1	3713.8	0.0
16	6H11/2	98.2	1	3766.1	0.0
17	6H11/2	98.6	1	3820.0	0.0
18	6H11/2	98.7	1	3861.0	0.0
19	6H13/2	99.0	1	4882.3	0.0
20	6H13/2	98.3	1	4977.6	0.0
21	6H13/2	97.7	1	5075.7	0.0
22	6H13/2	98.4	1	5111.6	0.0
23	6H13/2	97.8	1	5155.5	0.0
24	6H13/2	98.6	1	5191.0	0.0
25	6H13/2	98.2	1	5224.5	0.0
26	6H15/2	98.4	1	6267.1	0.0
27	6F 1/2	95.5	1	6364.0	0.0
28	6H15/2	96.2	1	6383.3	0.0
29	6H15/2	98.2	1	6447.3	0.0
30	6H15/2	97.4	1	6516.8	0.0
31	6H15/2	97.8	1	6574.9	0.0
32	6H15/2	93.4	1	6664.5	0.0
33	6F 3/2	91.4	1	6699.8	0.0
34	6F 3/2	75.5	1	6726.1	0.0
35	6H15/2	89.5	1	6741.6	0.0
36	6H15/2	85.1	1	6790.2	0.0
37	6F 5/2	97.2	1	7114.2	0.0
38	6F 5/2	94.4	1	7153.8	0.0
39	6F 5/2	96.7	1	7166.9	0.0

TABLE VIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR SmP_5O_{14}

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
40 6F 7/2	98.5	1	7967.4	0.0
41 6F 7/2	98.7	1	8009.0	0.0
42 6F 7/2	99.0	1	8026.5	0.0
43 6F 7/2	98.5	1	8063.8	0.0
44 6F 9/2	99.5	1	9107.9	0.0
45 6F 9/2	99.5	1	9134.2	0.0
46 6F 9/2	99.4	1	9179.4	0.0
47 6F 9/2	99.1	1	9194.1	0.0
48 6F 9/2	99.3	1	9219.2	0.0

TABLE IX. ENERGY LEVELS AND PHENOMENOLOGICAL B_{km} for Eu^{3+} IN EuP_5O_{14}[a]

```
EU IN P5014.  NEW ASSIGNMENTS BASED ON SCALED BKM FROM ND HOME.  9/22975.
FINAL  BKM AND CENTROIDS.  Q = 13.182
   -585.724 = B20    -212.651 = B22     -83.130 = B40    -751.307 = B42     -79.750 = B42
    131.526 = B60     117.952 = B62    -387.768 = B62      80.858 = B64     -67.600 = B64
7F 0          31.5
7F 1         405.1    111.358 = B44    -183.577 = B44
7F 2        1071.3    457.164 = B66       2.900 = B66
7F 3        1935.4
7F 4        2900.5
7F 5        3919.3
7F 6        5003.1
```

FREE ION		PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	7F 0	97.9	0	0.0	0.0
2	7F 1	99.2	0	272.1	271.0
3	7F 1	98.1	2	388.8	392.0
4	7F 1	97.4	2	476.3	474.0
5	7F 2	98.9	0	951.8	937.0*
6	7F 2	97.0	2	971.3	960.0
7	7F 2	97.5	2	1061.3	1070.0
8	7F 2	95.0	0	1091.7	1097.0
9	7F 2	95.8	0	1168.2	1180.0
10	7F 3	98.5	2	1854.8	1869.0*
11	7F 3	97.9	0	1886.2	1876.0
12	7F 3	94.6	2	1902.1	1890.0
13	7F 3	93.4	0	1911.9	1919.0
14	7F 3	97.0	2	1960.6	1928.0*
15	7F 3	94.7	0	1970.6	1982.0
16	7F 3	97.6	2	1991.2	2012.0*
17	7F 4	97.3	0	2742.2	2741.0
18	7F 4	95.5	2	2783.9	2794.0
19	7F 4	97.9	0	2833.6	2811.0*
20	7F 4	95.9	2	2837.4	2844.0
21	7F 4	96.5	0	2877.9	2869.0
22	7F 4	95.4	0	2969.2	2973.0
23	7F 4	97.4	2	2974.7	2979.0
24	7F 4	97.8	2	3002.5	3007.0
25	7F 4	97.8	0	3037.8	3040.0
26	7F 5	98.7	2	3754.2	3748.0
27	7F 5	98.1	2	3776.9	3774.0
28	7F 5	96.6	0	3839.7	3864.0*
29	7F 5	96.4	0	3900.7	3893.0
30	7F 5	94.8	0	3911.8	3907.0
31	7F 5	94.3	2	3919.3	3918.0
32	7F 5	97.3	2	3946.5	3929.0*
33	7F 5	98.5	2	3983.1	3984.0
34	7F 5	96.3	0	4006.2	4018.0
35	7F 5	97.4	0	4045.8	4049.0
36	7F 5	97.9	2	4059.4	4061.0
37	7F 6	99.2	0	4811.7	4798.0*
38	7F 6	99.1	0	4812.7	4811.0
39	7F 6	98.6	2	4907.4	4928.0*
40	7F 6	98.4	2	4913.4	4952.0*
41	7F 6	99.1	0	4966.4	4962.0
42	7F 6	99.2	2	4972.2	4980.0

[a]*The least-rms deviation between the calculated and experimental energy levels is 10.43 cm^{-1} (C. Brecher, J. Chem. Phys., 61 (1974), 2297).*

TABLE IX. ENERGY LEVELS AND PHENOMENOLOGICAL B_{km} FOR Eu^{3+} IN EuP_5O_{14}[a] (Cont'd)

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
43 7F 6	97.8	0	5024.2	4993.0*
44 7F 6	96.7	0	5047.6	5042.0
45 7F 6	97.0	2	5064.1	5057.0
46 7F 6	97.3	0	5145.6	5138.0
47 7F 6	97.5	2	5148.4	5160.0
48 7F 6	99.4	2	5266.6	5250.0*
49 7F 6	99.4	0	5266.9	5277.0

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[a] *The least-rms deviation between the calculated and experimental energy levels is 10.43 cm^{-1} (C. Brecher, J. Chem. Phys., 61 (1974), 2297).*

TABLE X. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR EuP_5O_{14}

```
EU IN EUP5014.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.   9/24/75.
INIT.  BKM AND CENTROIDS.  Q = -0.000
   -675.000 = B20      136.800 = B22     -140.400 = B40      696.100 = B42       81.700 = B42
    218.400 = B60     -114.300 = B62      340.900 = B62      245.000 = B64     -202.000 = B64
7F 0          96.0                        238.100 = B44     -352.800 = B44
7F 1         473.0                       -330.400 = B66      -49.000 = B66
7F 2        1175.0
7F 3        1998.0
7F 4        3000.0
7F 5        4073.0
7F 6        5094.0
5D 0    3  17220.0
5D 1    3  18960.0
5D 2    3  21422.0
5D 3    3  24653.0
```

FREE ION		PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	7F 0	97.6	0	61.1	0.0
2	7F 1	99.2	0	321.6	0.0
3	7F 1	97.6	2	478.7	0.0
4	7F 1	96.9	2	531.7	0.0
5	7F 2	96.7	2	1062.3	0.0
6	7F 2	98.1	0	1065.2	0.0
7	7F 2	96.9	2	1159.2	0.0
8	7F 2	93.5	0	1179.9	0.0
9	7F 2	95.9	0	1285.1	0.0
10	7F 3	98.2	2	1918.5	0.0
11	7F 3	97.3	0	1955.4	0.0
12	7F 3	95.1	2	1967.1	0.0
13	7F 3	92.2	0	1987.1	0.0
14	7F 3	96.8	2	2019.3	0.0
15	7F 3	94.3	0	2034.3	0.0
16	7F 3	96.7	2	2044.6	0.0
17	7F 4	97.4	0	2835.2	0.0
18	7F 4	95.3	2	2885.7	0.0
19	7F 4	97.4	0	2916.0	0.0
20	7F 4	95.7	2	2955.9	0.0
21	7F 4	96.2	0	3000.6	0.0
22	7F 4	96.2	0	3066.5	0.0
23	7F 4	97.5	2	3073.1	0.0
24	7F 4	97.7	2	3082.5	0.0
25	7F 4	97.5	0	3143.2	0.0
26	7F 5	98.4	2	3906.5	0.0
27	7F 5	97.9	2	3922.0	0.0
28	7F 5	94.9	0	4016.5	0.0
29	7F 5	96.6	0	4027.4	0.0
30	7F 5	93.2	2	4030.4	0.0
31	7F 5	94.5	0	4045.4	0.0
32	7F 5	97.9	2	4104.5	0.0
33	7F 5	97.7	2	4129.9	0.0
34	7F 5	96.5	0	4178.1	0.0
35	7F 5	97.5	0	4212.7	0.0
36	7F 5	98.3	2	4236.4	0.0
37	7F 6	99.2	0	4877.4	0.0
38	7F 6	99.0	0	4879.5	0.0
39	7F 6	98.2	2	4981.0	0.0
40	7F 6	98.0	2	4986.2	0.0
41	7F 6	98.2	0	5077.6	0.0
42	7F 6	98.2	2	5092.3	0.0
43	7F 6	96.3	0	5126.4	0.0

TABLE X. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR EuP_5O_{14} (Cont'd)

FREE ION	PCT	PURE	2MU	THEO.ENERGY	EXP.ENERGY
44 7F 6		96.5	0	5156.7	0.C
45 7F 6		96.6	2	519C.9	0.C
46 7F 6		98.0	2	5244.8	0.C
47 7F 6		98.0	0	5249.4	0.C
48 7F 6		99.4	2	5349.1	0.C
49 7F 6		99.4	0	5349.2	0.C
50 5D 0	3	100.0	0	17219.4	0.C
51 5D 1	3	100.0	0	1892C.9	0.C
52 5D 1	3	100.0	2	18968.9	0.C
53 5D 1	3	100.0	2	18988.6	0.C
54 5D 2	3	100.0	2	21401.2	0.C
55 5D 2	3	100.0	0	21404.2	0.C
56 5D 2	3	100.0	0	21418.5	0.C
57 5D 2	3	100.0	2	21439.8	0.C
58 5D 2	3	100.0	0	21445.2	0.C
59 5D 3	3	100.0	2	24618.2	0.C
60 5D 3	3	10C.0	2	24629.1	0.C
61 5D 3	3	100.0	0	24651.3	0.C
62 5D 3	3	100.0	0	24651.9	0.0
63 5D 3	3	100.0	2	24655.4	0.C
64 5D 3	3	100.0	0	24683.7	0.C
65 5D 3	3	100.0	2	24684.9	0.C

TABLE XI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR GdP_5O_{14}

```
GD IN GDP5O14.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.  9/24/75.
INIT.  BKM AND CENTROIDS.  Q = -0.000
   -646.200 = B20      131.000 = B22     -133.700 = B40     456.700 = B42    -487.100 = B42
    212.700 = B60     -346.300 = B62      -51.700 = B62     257.700 = B64    -170.700 = B64
8S 7/2          0.0
6P 7/2      32210.0    -276.800 = B44    -296.300 = B44
6P 5/2      32753.0    -304.200 = B66     114.900 = B66
6P 3/2      33289.0
6I 7/2      35865.0
6I 9/2      36217.0
6I17/2      36448.0
6I11/2      36516.0
6I13/2      36700.0
6I15/2      36711.0
```

	FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	8S 7/2	100.0	1	-0.4	0.0
2	8S 7/2	100.0	1	-0.2	0.0
3	8S 7/2	100.0	1	0.0	0.0
4	8S 7/2	100.0	1	0.3	0.0
5	6P 7/2	99.8	1	32137.7	0.0
6	6P 7/2	99.7	1	32177.6	0.0
7	6P 7/2	99.6	1	32213.5	0.0
8	6P 7/2	99.8	1	32272.0	0.0
9	6P 5/2	99.6	1	32713.0	0.0
10	6P 5/2	98.6	1	32733.9	0.0
11	6P 5/2	99.4	1	32777.5	0.0
12	6P 3/2	98.9	1	33261.1	0.0
13	6P 3/2	99.4	1	33299.3	0.0
14	6I 7/2	100.0	1	35842.9	0.0
15	6I 7/2	99.9	1	35863.6	0.0
16	6I 7/2	99.8	1	35877.7	0.0
17	6I 7/2	99.9	1	35886.9	0.0
18	6I 9/2	99.9	1	36188.9	0.0
19	6I 9/2	99.9	1	36205.0	0.0
20	6I 9/2	99.7	1	36225.4	0.0
21	6I 9/2	99.7	1	36231.3	0.0
22	6I 9/2	99.8	1	36245.3	0.0
23	6I17/2	98.6	1	36445.6	0.0
24	6I17/2	98.7	1	36445.7	0.0
25	6I17/2	99.3	1	36446.1	0.0
26	6I17/2	99.2	1	36446.2	0.0
27	6I17/2	99.0	1	36447.4	0.0
28	6I17/2	99.1	1	36448.3	0.0
29	6I17/2	98.2	1	36450.3	0.0
30	6I17/2	99.0	1	36453.5	0.0
31	6I17/2	99.1	1	36455.5	0.0
32	6I11/2	97.5	1	36485.5	0.0
33	6I11/2	97.9	1	36502.1	0.0
34	6I11/2	98.9	1	36511.1	0.0
35	6I11/2	98.6	1	36527.6	0.0
36	6I11/2	98.9	1	36535.8	0.0
37	6I11/2	98.9	1	36546.9	0.0
38	6I13/2	88.3	1	36666.0	0.0
39	6I13/2	98.6	1	36681.9	0.0
40	6I13/2	52.3	1	36686.4	0.0
41	6I13/2	52.0	1	36690.5	0.0
42	6I15/2	57.0	1	36693.6	0.0
43	6I15/2	82.6	1	36701.3	0.0
44	6I15/2	65.9	1	36706.8	0.0

TABLE XI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR GdP_5O_{14} (Cont'd)

FREE ION		PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
45	6I15/2	74.3	1	36710.6	0.0
46	6I15/2	54.3	1	36713.1	0.0
47	6I13/2	65.8	1	36717.5	0.0
48	6I13/2	55.9	1	36723.0	0.0
49	6I15/2	50.6	1	36726.3	0.0
50	6I15/2	79.3	1	36731.2	0.0
51	6I15/2	80.9	1	36741.8	0.0
52	6I15/2	57.0	1	36743.5	0.0

TABLE XII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR TbP_5O_{14}

```
TB IN TBP5C14.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.   9/24/75.
INIT.  BKM AND CENTRCIDS.  Q = -0.0C0
   -616.000 = B20      124.900 = B22     -126.700 = B40     -114.000 = B42     -622.500 = B42
    206.700 = B60       -9.200 = B62     -34C.200 = B62      266.500 = B64     -138.400 = B64
7F 6         310.0
7F 5        2347.0    -332.400 = B44      192.400 = B44
7F 4        3580.0    -203.900 = B66      241.500 = B66
7F 3        4573.0
7F 2        5155.0
7F 1        5432.0
7F 0        5766.0
5D 4   3   20569.0
5D 3   3   26357.0
```

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1 7F 6	99.6	2	88.8	0.C
2 7F 6	99.6	0	89.4	0.C
3 7F 6	99.3	0	17C.7	0.C
4 7F 6	99.1	2	192.7	0.C
5 7F 6	99.3	2	215.9	0.C
6 7F 6	99.6	0	265.6	0.C
7 7F 6	99.8	2	289.1	0.C
8 7F 6	99.0	0	311.1	0.C
9 7F 6	99.3	0	313.4	0.C
10 7F 6	99.8	2	441.6	0.C
11 7F 6	99.8	2	447.8	0.C
12 7F 6	99.8	0	515.8	0.C
13 7F 6	99.8	0	518.4	0.C
14 7F 5	98.7	2	2196.0	0.C
15 7F 5	98.6	0	2213.3	0.C
16 7F 5	97.9	0	2249.5	0.C
17 7F 5	98.9	2	2294.8	0.C
18 7F 5	96.7	0	2298.9	0.C
19 7F 5	98.6	2	2322.9	0.C
20 7F 5	99.2	0	2381.1	0.C
21 7F 5	98.7	2	2387.9	0.C
22 7F 5	98.7	0	2444.4	0.C
23 7F 5	99.1	2	2465.0	0.C
24 7F 5	99.4	2	2489.1	0.C
25 7F 4	97.8	0	3404.3	0.C
26 7F 4	97.6	2	3495.5	0.C
27 7F 4	95.2	0	3543.6	0.C
28 7F 4	97.7	2	3547.1	0.C
29 7F 4	97.3	2	3595.3	0.C
30 7F 4	99.3	0	3603.7	0.C
31 7F 4	99.6	0	3648.4	0.C
[illegible] 7F 4	97.1	2	3658.3	0.C
[illegible] 7F 4	98.0	0	3720.2	0.C
34 7F 3	97.0	2	4522.0	0.C
35 7F 3	91.5	0	4528.0	0.C
36 7F 3	95.7	2	4547.8	0.C
37 7F 3	96.4	0	4578.2	0.C
38 7F 3	92.5	0	4592.2	0.C
39 7F 3	95.2	2	4593.5	0.C
40 7F 3	97.7	2	4647.0	0.C
41 7F 2	93.4	0	5067.6	0.C
42 7F 2	91.5	2	5137.1	0.C
43 7F 2	91.2	0	5177.6	0.C
44 7F 2	94.9	0	5217.1	0.C
45 7F 2	80.8	2	5250.1	0.C
46 7F 1	80.8	2	5393.4	0.C
47 7F 1	89.9	2	5451.8	0.C
48 7F 1	98.0	0	5579.1	0.C

TABLE XII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR TbP_5O_{14} (Cont'd)

FREE ION			PCT	PURE	2MU	THEO.ENERGY	EXP.ENERGY
49	7F	0		94.0	0	5812.3	0.C
50	5D	4	3	100.0	0	20517.2	0.C
51	5D	4	3	100.0	2	20524.2	0.C
52	5D	4	3	100.0	0	20546.1	0.C
53	5D	4	3	100.0	2	20549.3	C.C
54	5D	4	3	100.0	0	20563.2	0.C
55	5D	4	3	100.0	2	20581.8	0.C
56	5D	4	3	100.0	2	20587.1	0.C
57	5D	4	3	100.0	0	20623.3	0.C
58	5D	4	3	100.0	0	20626.8	0.C
59	5D	3	3	100.0	2	26347.7	0.C
60	5D	3	3	100.0	0	26348.7	0.C
61	5D	3	3	100.0	0	26351.2	0.C
62	5D	3	3	100.0	2	26354.4	0.C
63	5D	3	3	100.0	2	26362.5	0.C
64	5D	3	3	100.0	2	26368.4	0.C
65	5D	3	3	100.0	0	26368.6	0.C

TABLE XIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR DyP_5O_{14}

DY IN DYP5O14. EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES. 9/24/75.
INIT. BKM AND CENTROIDS. Q = -0.000

-584.300 = B20	118.500 = B22	-119.300 = B40	-535.200 = B42	-262.000 = B42
200.600 = B60	323.500 = B62	-66.400 = B62	271.300 = B64	-107.000 = B64

6H15/2	262.0		
6H13/2	3710.0	106.800 = B44	345.700 = B44
6H11/2	6028.0	-58.800 = B66	301.100 = B66
6F11/2	7830.0		
6H 9/2	7879.0		
6F 9/2	9188.0		
6H 7/2	9243.0		
6H 5/2	10340.0		
6F 7/2	11071.0		
6F 5/2	12462.0		

	FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	6H15/2	100.0	1	32.7	0.0
2	6H15/2	99.9	1	137.8	0.0
3	6H15/2	99.9	1	176.0	0.0
4	6H15/2	99.9	1	230.2	0.0
5	6H15/2	99.9	1	262.2	0.0
6	6H15/2	99.9	1	311.5	0.0
7	6H15/2	99.9	1	378.4	0.0
8	6H15/2	99.9	1	508.0	0.0
9	6H13/2	99.9	1	3554.6	0.0
10	6H13/2	99.7	1	3622.6	0.0
11	6H13/2	99.6	1	3672.3	0.0
12	6H13/2	99.8	1	3686.2	0.0
13	6H13/2	99.6	1	3725.9	0.0
14	6H13/2	99.6	1	3798.0	0.0
15	6H13/2	99.7	1	3861.9	0.0
16	6H11/2	99.4	1	5923.2	0.0
17	6H11/2	99.2	1	5953.9	0.0
18	6H11/2	99.2	1	5971.9	0.0
19	6H11/2	99.4	1	6015.8	0.0
20	6H11/2	99.2	1	6093.6	0.0
21	6H11/2	99.5	1	6156.8	0.0
22	6F11/2	59.4	1	7704.5	0.0
23	6F11/2	49.7	1	7734.5	0.0
24	6F11/2	56.7	1	7767.0	0.0
25	6F11/2	52.8	1	7783.4	0.0
26	6F11/2	78.2	1	7810.5	0.0
27	6F11/2	73.1	1	7833.0	0.0
28	6F11/2	67.6	1	7872.3	0.0
29	6H 9/2	64.4	1	7900.9	0.0
30	6F11/2	65.1	1	7944.7	0.0
31	6H 9/2	70.7	1	7977.5	0.0
32	6H 9/2	66.7	1	8047.3	0.0
33	6F 9/2	53.6	1	9058.6	0.0
34	6H 7/2	58.9	1	9107.7	0.0
35	6F 9/2	62.3	1	9144.5	0.0
36	6F 9/2	87.3	1	9182.5	0.0
37	6F 9/2	87.9	1	9211.1	0.0
38	6F 9/2	78.8	1	9235.3	0.0
39	6H 7/2	63.5	1	9281.6	0.0
40	6H 7/2	61.9	1	9328.0	0.0
41	6H 7/2	83.9	1	9392.1	0.0

TABLE XIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR DyP_5O_{14} (Cont'd)

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
42 6H 5/2	96.9	1	10228.6	0.0
43 6H 5/2	97.7	1	10332.4	0.0
44 6H 5/2	95.3	1	10464.7	0.0
45 6F 7/2	97.6	1	11057.1	0.0
46 6F 7/2	99.1	1	11085.1	0.0
47 6F 7/2	97.5	1	11102.0	0.0
48 6F 7/2	98.7	1	11122.1	0.0
49 6F 5/2	99.6	1	12447.9	0.0
50 6F 5/2	99.8	1	12482.5	0.0
51 6F 5/2	99.6	1	12495.9	0.0

TABLE XIV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR HoP_5O_{14}

```
HO IN HOP5O14.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.  5/24/75.
INIT.  BKM AND CENTROIDS.  Q = -0.000
   -550.800 = B20      111.700 = B22     -111.400 = B40     -493.800 = B42      256.500 = B42
    194.300 = B60      117.900 = B62      297.400 = B62      272.200 = B64      -75.600 = B64
5I 8        169.6
5I 7       5219.5      337.000 = B44      -25.000 = B44
5I 6       8717.6       92.300 = B66      282.500 = B66
5I 5      11274.7
5I 4      13333.4
```

FREE ION			PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	5I	8	100.0	0	17.0	0.0
2	5I	8	100.0	2	18.9	0.0
3	5I	8	100.0	2	31.4	0.0
4	5I	8	100.0	0	40.7	0.0
5	5I	8	100.0	0	69.1	0.0
6	5I	8	100.0	2	102.6	0.0
7	5I	8	100.0	0	138.4	0.0
8	5I	8	100.0	2	167.3	0.0
9	5I	8	100.0	0	170.2	0.0
10	5I	8	100.0	2	201.6	0.0
11	5I	8	100.0	0	226.8	0.0
12	5I	8	100.0	0	246.9	0.0
13	5I	8	100.0	2	247.3	0.0
14	5I	8	100.0	2	275.8	0.0
15	5I	8	100.0	2	286.3	0.0
16	5I	8	100.0	0	303.3	0.0
17	5I	8	100.0	0	306.6	0.0
18	5I	7	100.0	0	5138.6	0.0
19	5I	7	100.0	2	5138.7	0.0
20	5I	7	100.0	2	5183.1	0.0
21	5I	7	99.9	0	5183.3	0.0
22	5I	7	99.9	2	5197.2	0.0
23	5I	7	99.9	0	5197.7	0.0
24	5I	7	99.9	2	5205.0	0.0
25	5I	7	100.0	0	5205.0	0.0
26	5I	7	99.9	2	5228.3	0.0
27	5I	7	99.9	0	5232.5	0.0
28	5I	7	99.9	2	5240.4	0.0
29	5I	7	99.9	0	5268.2	0.0
30	5I	7	99.9	0	5269.7	0.0
31	5I	7	99.9	2	5295.3	0.0
32	5I	7	100.0	2	5296.4	0.0
33	5I	6	99.9	2	8639.8	0.0
34	5I	6	99.9	0	8640.7	0.0
35	5I	6	99.9	0	8689.3	0.0
36	5I	6	99.9	2	8692.5	0.0
37	5I	6	99.9	2	8705.5	0.0
38	5I	6	99.8	0	8708.3	0.0
39	5I	6	99.8	0	8715.4	0.0
40	5I	6	99.8	2	8720.4	0.0
41	5I	6	99.9	0	8735.0	0.0
42	5I	6	99.8	2	8745.9	0.0
43	5I	6	99.8	2	8751.4	0.0
44	5I	6	99.9	0	8788.5	0.0
45	5I	6	99.9	0	8790.0	0.0
46	5I	5	99.7	0	11209.3	0.0
47	5I	5	99.9	2	11211.4	0.0
48	5I	5	99.8	0	11254.2	0.0
49	5I	5	99.6	2	11256.7	0.0
50	5I	5	99.8	2	11265.3	0.0
51	5I	5	99.7	0	11269.2	0.0
52	5I	5	99.9	2	11285.4	0.0
53	5I	5	99.5	0	11288.4	0.0
54	5I	5	99.8	0	11305.7	0.0

TABLE XIV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR HoP_5O_{14} (Cont'd)

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
55 5I 5	99.5	2	11332.2	0.C
56 5I 5	99.9	2	11341.1	0.C
57 5I 4	99.8	0	13244.2	0.C
58 5I 4	99.7	2	13244.6	0.C
59 5I 4	99.8	0	13285.0	0.C
60 5I 4	99.5	0	13298.7	0.C
61 5I 4	99.5	2	13328.1	0.C
62 5I 4	99.8	2	13336.7	0.C
63 5I 4	99.9	2	13426.9	0.C
64 5I 4	99.8	0	13427.6	0.C
65 5I 4	100.0	0	13462.8	0.C

TABLE XV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR ErP_5O_{14}

```
ER IN ERP5014.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.  9/24/75.
INIT.  BKM AND CENTROIDS.  Q = -0.000
   -515.000 = B20     104.400 = B22    -102.900 = B40      -80.600 = B42     507.700 = B42
    187.800 = B60    -263.100 = B62     162.300 = B62      269.300 = B64     -45.200 = B64
4I15/2      263.0
4I13/2     6736.0      47.200 = B44    -308.500 = B44
4I11/2    10346.0     210.800 = B66     195.100 = B66
4I 9/2    12560.0
4F 9/2    15365.0
4S 3/2    18444.0
2H11/2 2  19190.0
4F 7/2    20582.0
4F 5/2    22230.0
4F 3/2    22561.0
```

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1 4I15/2	100.0	1	87.5	0.0
2 4I15/2	100.0	1	119.0	0.0
3 4I15/2	100.0	1	199.3	0.0
4 4I15/2	100.0	1	251.7	0.0
5 4I15/2	100.0	1	306.1	0.0
6 4I15/2	100.0	1	337.9	0.0
7 4I15/2	100.0	1	369.6	0.0
8 4I15/2	100.0	1	413.5	0.0
9 4I13/2	100.0	1	6632.6	0.0
10 4I13/2	99.9	1	6668.6	0.0
11 4I13/2	99.9	1	6717.9	0.0
12 4I13/2	99.9	1	6733.3	0.0
13 4I13/2	100.0	1	6782.0	0.0
14 4I13/2	100.0	1	6795.0	0.0
15 4I13/2	100.0	1	6808.2	0.0
16 4I11/2	99.9	1	10289.2	0.0
17 4I11/2	99.9	1	10316.4	0.0
18 4I11/2	99.9	1	10340.7	0.0
19 4I11/2	99.9	1	10363.9	0.0
20 4I11/2	99.9	1	10372.1	0.0
21 4I11/2	100.0	1	10389.6	0.0
22 4I 9/2	99.9	1	12458.6	0.0
23 4I 9/2	99.9	1	12477.0	0.0
24 4I 9/2	100.0	1	12585.7	0.0
25 4I 9/2	100.0	1	12612.5	0.0
26 4I 9/2	100.0	1	12661.7	0.0
27 4F 9/2	99.9	1	15289.2	0.0
28 4F 9/2	100.0	1	15344.6	0.0
29 4F 9/2	100.0	1	15362.0	0.0
30 4F 9/2	99.9	1	15407.1	0.0
31 4F 9/2	99.9	1	15428.3	0.0
32 4S 3/2	99.3	1	18409.0	0.0
33 4S 3/2	98.9	1	18468.4	0.0
34 2H11/2 2	99.7	1	19144.8	0.0
35 2H11/2 2	99.3	1	19164.0	0.0
36 2H11/2 2	99.7	1	19168.3	0.0
37 2H11/2 2	99.6	1	19198.9	0.0
38 2H11/2 2	99.2	1	19223.8	0.0
39 2H11/2 2	99.5	1	19250.2	0.0
40 4F 7/2	99.8	1	20515.6	0.0
41 4F 7/2	99.5	1	20563.8	0.0
42 4F 7/2	99.5	1	20598.1	0.0
43 4F 7/2	99.7	1	20665.4	0.0

TABLE XV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR ErP_5O_{14} (Cont'd)

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
44 4F 5/2	98.5	1	22210.3	0.0
45 4F 5/2	97.6	1	22222.8	0.0
46 4F 5/2	99.4	1	22258.3	0.0
47 4F 3/2	98.1	1	22527.0	0.0
48 4F 3/2	97.7	1	22615.0	0.0

TABLE XVI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR TmP_5O_{14}

```
TM IN TMP5O14.  EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES.  3/24/75.
INIT.  BKM AND CENTROIDS.  C = -0.000
   -476.600 = B20      96.600 = B22     -93.700 = B40      329.000 = B42      333.600 = B42
    181.100 = B60    -198.300 = B62    -222.500 = B62      262.700 = B64      -16.200 = B64
3H 6        255.0
3F 4       5820.0    -264.000 = B44    -104.700 = B44
3H 5       8435.0     269.100 = B66      65.300 = B66
3H 4      12731.0
3F 3      14529.0
3F 2      15133.0
1G 4      21325.0
1D 2      27892.0
```

FREE ION		PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	3H 6	100.0	0	-1.3	0.0
2	3H 6	100.0	0	9.3	0.0
3	3H 6	100.0	2	143.9	0.0
4	3H 6	100.0	2	170.7	0.0
5	3H 6	100.0	0	242.2	0.0
6	3H 6	100.0	2	252.7	0.0
7	3H 6	100.0	0	285.7	0.0
8	3H 6	100.0	0	319.0	0.0
9	3H 6	100.0	2	330.7	0.0
10	3H 6	100.0	2	346.9	0.0
11	3H 6	100.0	0	351.8	0.0
12	3H 6	99.9	2	408.4	0.0
13	3H 6	99.9	0	410.3	0.0
14	3F 4	99.8	2	5691.8	0.0
15	3F 4	99.6	0	5712.5	0.0
16	3F 4	99.8	0	5779.7	0.0
17	3F 4	99.7	2	5787.3	0.0
18	3F 4	99.9	0	5827.5	0.0
19	3F 4	99.9	2	5842.5	0.0
20	3F 4	100.0	0	5874.3	0.0
21	3F 4	99.9	0	5917.5	0.0
22	3F 4	99.9	2	5927.4	0.0
23	3H 5	100.0	2	8243.8	0.0
24	3H 5	99.8	2	8251.2	0.0
25	3H 5	99.7	0	8375.5	0.0
26	3H 5	99.9	0	8379.6	0.0
27	3H 5	99.9	2	8451.2	0.0
28	3H 5	99.9	0	8471.6	0.0
29	3H 5	99.9	2	8474.8	0.0
30	3H 5	99.8	0	8513.7	0.0
31	3H 5	99.9	2	8514.0	0.0
32	3H 5	99.8	2	8554.2	0.0
33	3H 5	99.9	0	8556.3	0.0
34	3H 4	99.6	0	12547.4	0.0
35	3H 4	100.0	0	12610.5	0.0
36	3H 4	99.6	2	12671.9	0.0
37	3H 4	99.6	0	12751.2	0.0
38	3H 4	99.8	2	12757.8	0.0
39	3H 4	99.8	2	12765.2	0.0
40	3H 4	99.8	0	12792.7	0.0
41	3H 4	99.6	2	12815.1	0.0
42	3H 4	99.6	0	12830.0	0.0
43	3F 3	99.3	0	14490.8	0.0
44	3F 3	99.6	2	14494.9	0.0
45	3F 3	99.3	0	14515.1	0.0
46	3F 3	99.7	2	14534.1	0.0
47	3F 3	99.3	0	14553.7	0.0
48	3F 3	99.7	2	14559.2	0.0
49	3F 3	99.5	2	14592.6	0.0

TABLE XVI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR TmP_5O_{14}(Cont'd)

FREE ION			PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
50	3F	2	99.2	0	15083.4	0.C
51	3F	2	99.6	2	15085.9	0.C
52	3F	2	99.2	2	15133.7	0.C
53	3F	2	99.6	0	15176.8	0.C
54	3F	2	99.8	0	15225.3	C.C
55	1G	4	100.C	2	2116C.6	0.C
56	1G	4	10C.0	0	21167.9	0.C
57	1G	4	10C.0	0	21252.7	0.C
58	1G	4	100.0	2	21312.3	0.C
59	1G	4	100.0	0	21313.9	0.C
60	1G	4	10C.0	2	21344.2	0.C
61	1G	4	100.C	0	21385.8	0.C
62	1G	4	100.0	0	21484.9	0.C
63	1G	4	100.0	2	21511.7	0.C
64	1D	2	100.0	0	27822.8	0.C
65	1D	2	10C.0	2	27837.9	0.C
66	1D	2	100.0	2	27885.6	0.C
67	1D	2	10C.0	0	27957.9	0.C
68	1D	2	10C.C	0	2797C.5	0.C

TABLE XVII. AMPLITUDES, A_{km}, IN CM^{-1} $\mathring{A}^{-k}$, OF SPHERICAL DECOMPOSITION OF LATTICE SUMS FOR NdP_5O_{14}†

k	m	A_{km} (q_0 = -1)‡		A_{km} (q_0 = -2)‡	
		Real	Imaginary	Real	Imaginary
1	0	16797.4	0	23799.2	0
1	1	-37138.	5876.2	-69989.6	12348.9
2	0	-3006.66	0	-5414.44	0
2	1	24.0762	-210.429	32.735	-440.936
2	2	-46.2236	-699.385	-476.544	-742.301
3	0	146.631	0	272.599	0
3	1	113.903	-113.566	245.472	174.387
3	2	23.9621	118.058	23.3478	221.346
3	3	-107.	206.525	-512.996	235.769
4	0	1459.8	0	2659.56	0
4	1	-104.684	-153.643	-210.048	-308.525
4	2	-1196.65	985.944	-2418.41	1926.86
4	3	194.779	9.65227	400.361	21.1591
4	4	-658.119	-1337.65	-1156.92	-2600.78
5	0	-4.45292	0	-8.32774	0
5	1	759.959	-413.245	1502.53	-818.815
5	2	-33.9232	-12.0518	-69.3783	-25.2627
5	3	55.5247	-1357.2	124.874	-2646.4
5	4	74.1133	-34.314	148.632	-68.9808
5	5	-267.703	-218.441	-554.059	-448.519
6	0	202.617	0	403.34	0
6	1	2.44617	23.9365	5.33098	48.019
6	2	-95.8561	130.302	-189.637	258.726
6	3	-11.6831	-17.1279	-22.8872	-34.8373
6	4	-52.1825	-134.274	-116.977	-267.059
6	5	-12.6303	10.3804	-25.5546	20.0073
6	6	206.515	22.0685	411.215	43.7949
7	0	4.1059	0	8.26562	0
7	1	-47.8198	51.1209	-94.1572	101.206
7	2	-5.24923	-7.26414	-10.3708	-14.4391
7	3	-3.467	-15.118	-6.88997	-30.8619
7	4	4.838	1.1332	9.7122	2.29936
7	5	-25.74	-28.179	-51.1031	-56.7309
7	6	1.327	10.5704	2.61491	21.295
7	7	-32.06	20.2109	-64.6403	39.2683

†*Lattice constants are a = 8.771 Å, b = 9.012 Å, c = 13.057 Å, and β = 89.58 deg (H. Y-P. Hong, Acta Crystallogr., B30 (1974), 468).*

‡*Oxygen charge, q_O. Neodymium and phosphorus charges taken as q_{Nd} = +3, $q_P = -(3 + 14q_O)/5$.*

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